



**Y-12
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Explosive Potential Analysis of AB Process – Final Report

J. S. Bullock

Chemistry and Chemical Engineering Department
Technology Development Organization
Y-12 National Security Complex

**G. E. Giles, Jr.
M. W. Wendel**

Computational Modeling and Simulation Section
Computational Physics & Engineering Division
Oak Ridge National Laboratory

C. D. Sulfredge

Engineering Science Section
Engineering Technology Division
Oak Ridge National Laboratory

Issue Date: October 12, 2001

Prepared by the
Y-12 National Security Complex
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INTRODUCTION & SUMMARY

A need arose to define the hazards associated with the operation of a process. The process involved the evolution of a hydrogen gas stream from thermal decomposition of uranium hydride at approximately 400°C into the interior of a purged argon-filled glove box. Specific hazards of interest included the potential reaction severity of the evolved hydrogen with atmospheric oxygen, either downstream in the vent system or inside the box in the event of serious air inleakage. Another hazard might be the energetic reaction of inleaked air with the hot uranium and uranium hydride powder bed, possibly resulting in the dispersion of powders into an air atmosphere and the rapid combustion of the powders. This was approached as a problem in calculational simulation. Given the parameters associated with the process and the properties of the glove box system, certain scenarios were defined and the potential for flammable or detonation reactions estimated. Calculation tools included a comprehensive fluid dynamics code, a spreadsheet, a curve-fitting program, an equation solver, and a thermochemistry software package. Results are reported which suggest that the process can be operated without significant hazard to operators or significant damage to equipment, assuming that operators take account of potential upset scenarios.

Characteristics of the Process

The glovebox dimensions are: a length of 97 inches, a maximum (bottom) depth of 26 inches, a maximum (rear) height of 34 inches; and a front height of 12 inches and top depth of 14 inches which defines the sloping front for the window. This box has a total interior volume of 71,000 cubic inches (1,163.5 L). In normal operation an inflow of argon purges the box at a rate of 10 ft³/hr (4.72 L/min), and an oxygen monitor stream is removed at a rate of 3 ft³/hr (1.416 L/min). One parameter change during the process may be the increase of the argon purge rate to as high as 50 ft³/hr (23.60 L/min).

A small tube furnace, vertically oriented, is positioned in the center bottom of the glovebox. A reaction tube 1.5 inches inside diameter is located in the furnace with the outlet at a height of 22 inches above the glovebox floor. The reaction tube is made from MgO ceramic and has wall thickness of 0.25 inches and a spherical contour closed end. A charge of 250g UH₃ is assumed. Hydrogen gas is released across a surface 4 to 8 inches deep inside the reaction tube, which was nominally given a temperature of 400°C. The reaction proceeds according to the stoichiometry:



where the literature data for equilibrium pressureⁱ indicates a pressure of 0.510 atm at 400°C and 0.791 atm at 420°C . This is an endothermic reaction, requiring the supply of furnace heat to exactly balance the positive reaction enthalpy in order to maintain a constant process temperature.

Thermogravimetric analysesⁱⁱ reveal that at 400°C the rate of decomposition is such as to evolve, for this size of charge, 2.5 mg/s H₂ gas. At this temperature and for this tube cross-section, this is equivalent to 68.5 cc/s, or a velocity of 6.0 cm/s away from the bed. The total hydrogen evolved for this size charge is 1.556 moles H₂. For these simulations, the evolution rate was given values from 1.433 to 9.164 mg/s.

Calculation Scenarios

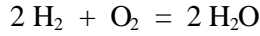
- 1) No ventilation in the box, all hydrogen evolved into the box, full mixing.
- 2) Hydrogen evolved into the box with 50 ft³/hr argon purge and 3 ft³/hr argon extraction to the oxygen monitor.
- 3) Hydrogen evolved into the box with 10 ft³/hr argon purge and 3 ft³/hr argon extraction to the oxygen monitor.
- 4) Hydrogen evolved into the box with 20 ft³/hr purge rate and 3 ft³/hr argon extraction to the oxygen monitor.
- 5) Hydrogen evolved into the box, no argon purge or extraction to oxygen monitor, gas leaves purge exit port at same volumetric rate as hydrogen generation rate.
 - A) complete mixing prior to exiting box (analytical solution)
 - B) mixing simulated by CFX, using 2.866 and 9.164 mg/s evolution rates
- 6) Hydrogen evolved into the box, no argon purge or extraction to oxygen monitor, one glove port becomes fully open.
 - A) Glove port opening occurs after significant hydrogen has been evolved
 - B) Air mixes with evolving hydrogen to form flammable/detonable mixtures
 - C) Air transports smoothly to powder bed to potentially accelerate reactions
 - D) Air transports in a burst to powder bed and initiates rapid reaction that throws powder out into glovebox space.
- 7) Separate calculation of consequences of Scenario 6D.

Calculation Tools

Excel 97 (MicroSoft), TK Solver Ver. 3.32 (Universal Technical Systems) and TableCurve 2D (Jandel Scientific) were used to manipulate values, determine reaction stoichiometries, curvefit data, and perform conversions from, for example, mass fraction to mole fraction. The fluid dynamics calculations were done using CFX-5, a product of AEA Technology Engineering Software Division. This code can deal with multiple gases, arbitrary flows, buoyancy changes due to temperature, heat transfer, and both diffusion and convection phenomena. One very sophisticated feature of CFX that was applied to this problem is the ability to calculate spatial maps of functional relationships between values of calculated parameters. This was applied to a function of the simultaneous presence of oxygen and hydrogen. Thermodynamic calculations on possible reactions that may occur between air and the hot powder bed were done using HSC Chemistry Ver. 4.0, a product of Outokumpu Research Oy, Finland.

Theory and Parameter Conversions

The reaction between hydrogen and oxygen occurs with the following stoichiometry:



Thus, from a mass transport perspective two hydrogen molecules must be delivered to the reaction site for every oxygen molecule. It is known that mixtures with this ratio yield the highest energy release. The kinetics of the hydrogen-oxygen reaction are actually rather complex, and cannot be explicitly incorporated into the present analysis at this time. However, an approximate expression such as the following should be valid:

$$R = k * [\text{H}_2]^2 * [\text{O}_2],$$

Where the reaction rate R is equal to the product of an overall rate constant k times the square of the hydrogen concentration times the oxygen concentration. This is consistent with a published kinetic expression for the hydrogen-oxygen reactionⁱⁱⁱ. The rate at which the reaction becomes a self-propagating flame or a self-propagating detonation relates to the concentration of the two reactants. For example, in a mixture with air, hydrogen reaches the lower flammability limit (LFL) at a concentration of 4 volume percent and reaches the lower explosion limit (LEL) at a concentration of 18.3 volume percent^{iv}. While adding a diluent such as argon to the mixture can be expected to affect the LFL and LEL due to changes in the thermal conductivity of the medium (carrying away energy which would otherwise be used to raise the reaction rate of mixtures ahead of the reaction front), to a first approximation it is useful to take the LFL and LEL concentration products as criteria for the limits for the hydrogen/air/argon system. We will use the mole fraction concentration system (for an ideal gas this is equivalent to the volume fraction) and assume a pressure of 1 atmosphere.

Thus, the criterion for the LFL will be taken as:

$$F_p = [\text{H}_2]^2 * [\text{O}_2] = [0.04]^2 * (1 - 0.04) * [0.21] = 0.0003226$$

and the criterion for the LEL will be taken as:

$$F_p = [\text{H}_2]^2 * [\text{O}_2] = [0.183]^2 * (1 - 0.183) * [0.21] = 0.005746$$

In other words, whenever the mole fraction product for the hydrogen and oxygen concentrations reaches 0.0003226 or above, a self-propagating flame is possible. Whenever the product reaches 0.005746 or above, a detonation is possible. It should be noted that this will be most accurate for the hydrogen-poor region. If one were to take the upper flammability and upper explosability limits^{iv} to create similar criteria, they would be less restrictive; hence, use of LFL and LEL to create such criteria is conservative.

The CFX code produces output as mass fractions of all input species for positions in space and as a function of time. The code can also calculate functional relationships between these concentrations and create maps of regions in space that have certain values of such functions. In order to make comparisons to the LFL and LEL criteria above, conversions of mass fraction to mole fraction must be done; this can also be done within CFX.

For example, the mass fraction of hydrogen is defined as:

$$\text{MFH}_2 = (\text{gH}_2/\text{cc}) / ((\text{gH}_2/\text{cc}) + (\text{gAir}/\text{cc}) + (\text{gAr}/\text{cc}))$$

Mass fractions can be manipulated to yield the mole fraction hydrogen as follows:

$$X_{H_2} = (MF_{H_2} / 2) / ((MF_{H_2} / 2) + (MF_{Air} / 29) + (MF_{Ar} / 40)) ,$$

Where the divisors 2, 29 and 40 are the molecular weights for hydrogen, air and argon respectively. The mole fraction air is determined by a similar calculation and then the oxygen mole fraction is determined as 0.21 times the air mole fraction.

Results for Calculation Scenarios

Scenario (1): If the full 1.556 moles hydrogen is evolved into the box and complete mixing occurs, the final mixture has a composition of 3.27 volume % hydrogen. Mixtures of 8% hydrogen in argon are commonly supplied as non-flammable gas, and the actual level at which the mixture is flammable is probably above 10%. Thus a uniform mixture at this level presents no reaction hazard.

Scenario (2): With a full 50 ft³/hr argon leaving the box, and a hydrogen production rate of 1.433 mg/s, if all the hydrogen were to be directed into the exit streams the hydrogen content of the exit streams would be 4.26 volume %. If full mixing were to occur before leaving the box, a steady-state exit concentration much lower would result. CFX calculation results of this for two evolution rates are shown in Table 1. It is noted, without interpretation at this time, that the exit concentration appears to be roughly proportional to the square of the hydrogen evolution rate.

Table 1 – Hydrogen Concentration at the Exit during the Process while Operating Normally

H ₂ Evolution Rate (mg/s)	Time after Evolution Start (s)	Mass Fraction H ₂	Volume % H ₂
1.433	93.5	6.663*10 ⁻⁷	0.00132
1.433	245	1.075*10 ⁻⁵	0.02132
2.866	288	4.316*10 ⁻⁵	0.08546
2.866	300	4.750*10 ⁻⁵	0.09404

Scenario (3): Reducing this purge to 10 ft³/hr, and again considering all the hydrogen to directly exit the box with no mixing, would yield a hydrogen content in the exit stream of 18.14 volume %, which would most likely be flammable. However, CFX results indicate that, for the 1.433 mg/s rate, the dilution which occurs prior to being included in the exiting gas would reduce this concentration to a mass fraction of 6.561*10⁻⁶, or 0.01302 vol %, at the 195 s mark.

Scenario (4): If the purge is made 20 ft³/hr, the exit hydrogen concentration would be 10 volume % with the above no-mixing assumption. This would most likely not be flammable. There are no CFX results for this case, but comparison with the 10 and 50 ft³/hr cases indicate a probable concentration in the range of 0.02 vol % for the 1.433 mg/s case and 0.08 vol % for the 2.866 mg/s case.

Scenario (5a): The concentration of hydrogen in the box will exponentially approach a value lower than in scenario (1). As hydrogen builds up in the box, and assuming complete mixing prior to exiting the box, the proportion of hydrogen in the exit gas will increase. The amount of hydrogen remaining in the box at any time t (minutes) would be:

$$\text{Moles H}_2 = (1 - \exp(-0.021026 * (dH_2/dt) * t)) / (0.021026)$$

At a constant evolution rate dH_2/dt of 1.24 mmole/s (2.5 mg/s), evolution would be complete in 20.9 minutes. At that time, there would be 1.5309 moles hydrogen in the box, or 98.4 % of all the hydrogen evolved. This is equivalent to 3.22 % hydrogen in the argon. Because (at a constant evolution rate) the product of the evolution rate and the time-to-completion is constant, the final concentration would be the same for any evolution rate (given the complete mixing assumption) and only depends on the total amount evolved.

Scenario (5b): However, mixing will probably not be complete due the buoyancy of the hydrogen causing it to tend to rise to the top of the box, where the exit port is located. Thus, a higher concentration will occur in the exit line and a lower concentration lower in the box. However, CFX calculations as presented below indicate that the exit line concentration will not be in the flammable range when mixed with air.

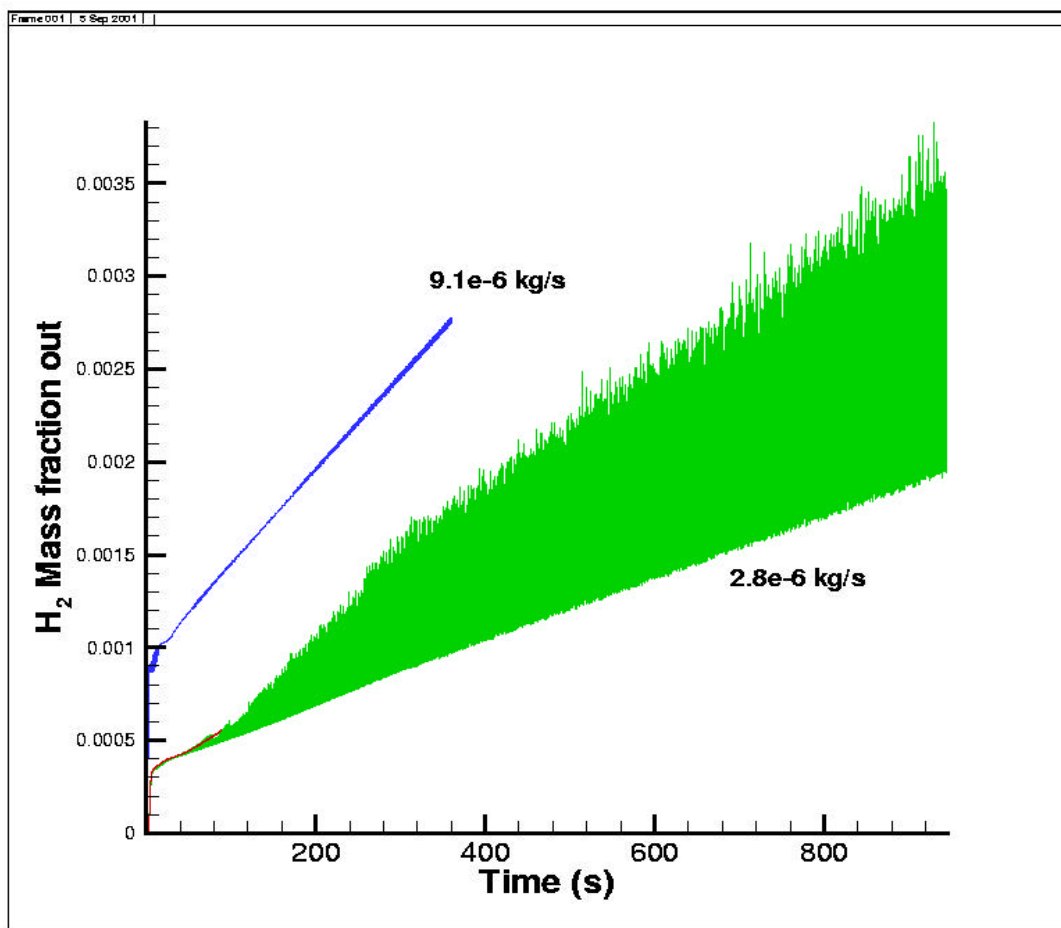


Figure 1 - H_2 Concentration at the Exit for Zero Ar Flow and Two Production Rates (c_H2MF_out_ta.cps)

Figure 1 shows the simulated hydrogen concentration (in argon) at the purge exit for two hydrogen production rates, assuming zero argon purge. The simulation for 2.866 mg/s was run using a time step of 0.1 s. This calculation yielded a bistable result, with a fairly linear baseline and an irregular upper branch (this plot is deceiving, as the middle part is occupied by connecting lines and not data points). At this production rate, the process would be complete in 1100 s. Projection of the curvefit for the mean of all the data points to 1100 s yields a prediction of 5.27 vol % hydrogen. Barely visible is a run at the same

production rate that used a time step of 0.01 s , terminating at 90 s, and that is rather free of noise. This shows more of a similarity to the upper branch of the data; however, with the changes in the upper branch that occur after about 100 s, there is no assurance that this similarity would continue to hold. The case can be made that this run with 0.01 s time steps might actually follow the mean as noted above. If the “true” value did indeed follow the upper branch (and there is good reason to doubt that), the final hydrogen concentration would be 7.09 vol %, still lower than the flammable limit.

The simulation for 9.164 mg/s was run using a time step of 0.25 s, and is quite stable. Normally, shorter time steps improve solution stability and longer steps increase instability. However, the increased hydrogen generation rate seems to stabilize the calculation. This run would be over at 347 s at this production rate. Projection of the calculation to this time yields a value of 5.44 vol %, only slightly higher than the rate predicted by the projection of the mean values for the 2.866 mg/s data. This is consistent with reasonable expectations.

The general conclusion from this set of calculations is that in the range from 2.866 to 9.164 mg/s hydrogen production rate, it is not possible to exceed the limit for flammability of the hydrogen-argon mixture in air as it exits the box.

Scenario 6A: No argon purge, hydrogen generation for an interval, then open a glove port. Figure 2 shows CFX output for the case where hydrogen is evolved for 105 s, then the glove port opens and 95 more seconds passes. What is shown is the streamlines associated with air ingress into the glovebox. There is a complementary view of argon egressing the box, which is not shown.

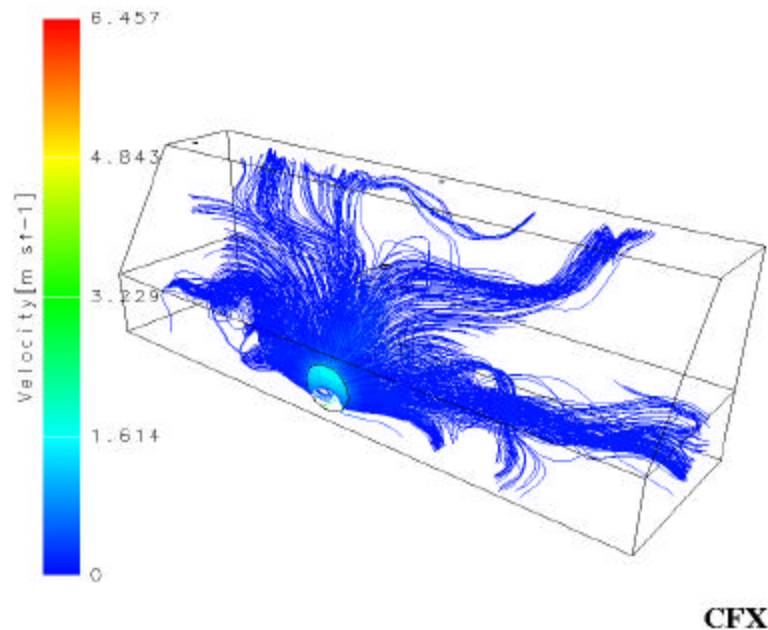


Figure 2 - CFX – Calculated Streamlines for Ingress of Air after Opening Glove Port (str_go_200s.ps)

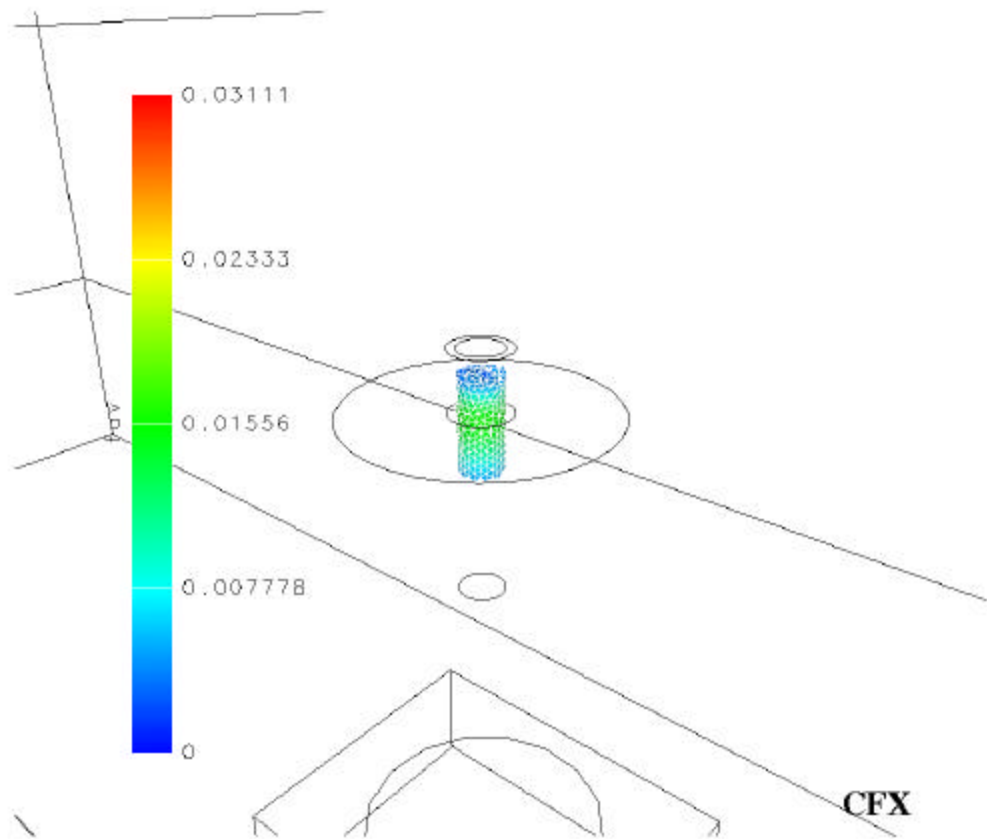


Figure 3 - Relatively Low Detonable Volume (iso_f_400s_92s.ps)

Scenario 6B: The set of figures from Fig. 3-5 illustrates the volume which meets the detonability criterion ($F_p \geq 0.005746$) for the case where the H_2 production rate is 2.866 mg/s , the argon flow is off, and the glove port has been opened to the air. The particular moment in time for Figure 3 is 92 seconds after opening the glove port and 400 seconds after starting hydrogen generation (see the correspondence with the file name appended to the figure legend).

Note that the detonable volume is still relatively small. Note also that there is a region, between the disk that is the source of hydrogen and the lower surface of the detonable region, where the gas mixture is too rich to be detonable. All the simulations of this type, which demonstrate behavior over the powder bed (and indeed the later calculations which examine the reaction of air with the powder bed), are based on an 8-inch headspace between the powder bed and the crucible outlet. The most recent information indicates that a different geometry will be used which gives a 4-inch headspace over the powder. A smaller headspace reduces the total volume of potential explosive gas mixtures (the headspace volume is a significant fraction of the total), and thus the calculated results reported here are more conservative than the actual situations.

The complete set of runs vs time demonstrates oscillatory behavior (see Figs. 6-7). This is a result of low-density hydrogen appearing inside a tube and below a higher-density air-argon mixture. Such bubbling is a physically reasonable result and does not indicate calculational solution instability.

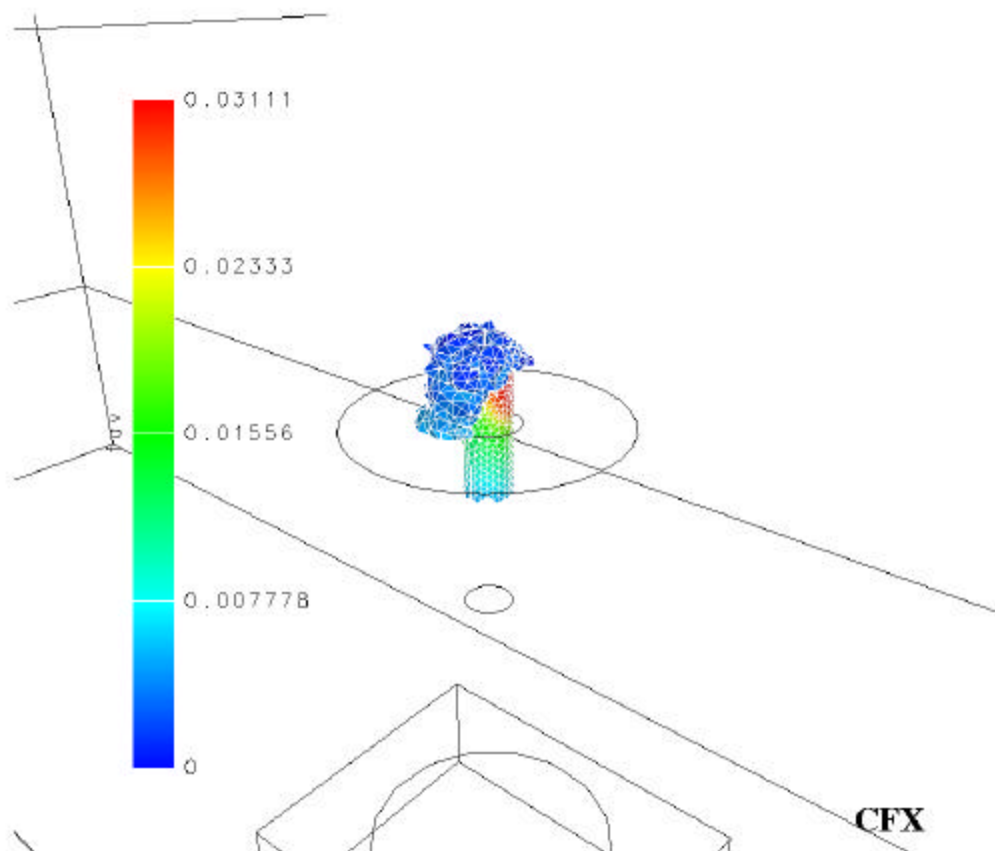


Figure 4 - Relatively High Detonable Volume (iso_f_1000s_692s.ps)

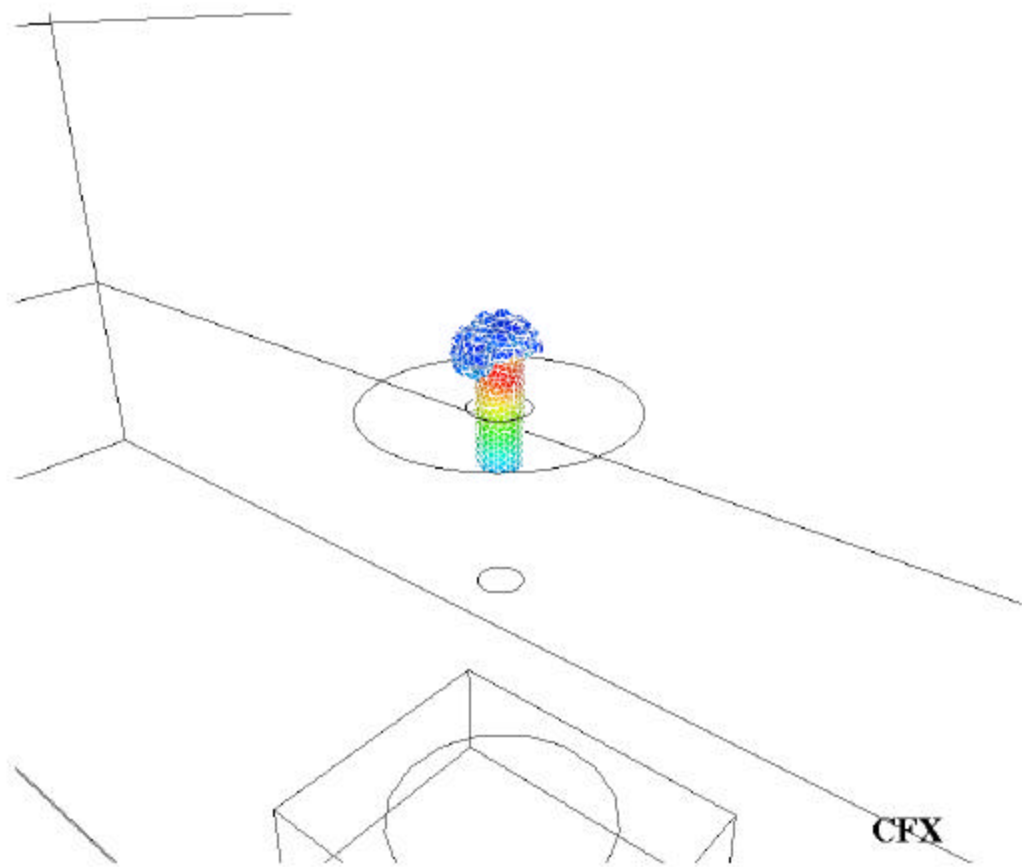


Figure 5 - Typical Detonable Volume (iso_f_1500s_1192s.ps)

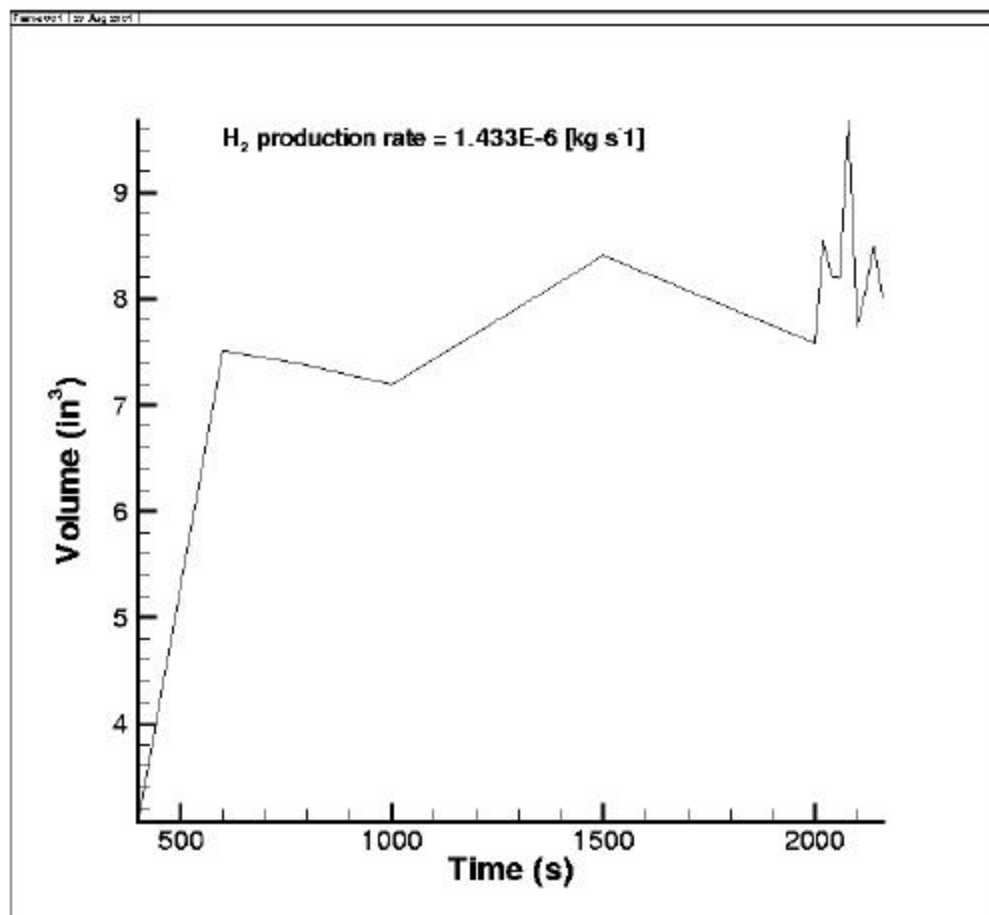


Figure 6 - Variation in Detonable Volume Size for Lower H_2 Production Rate

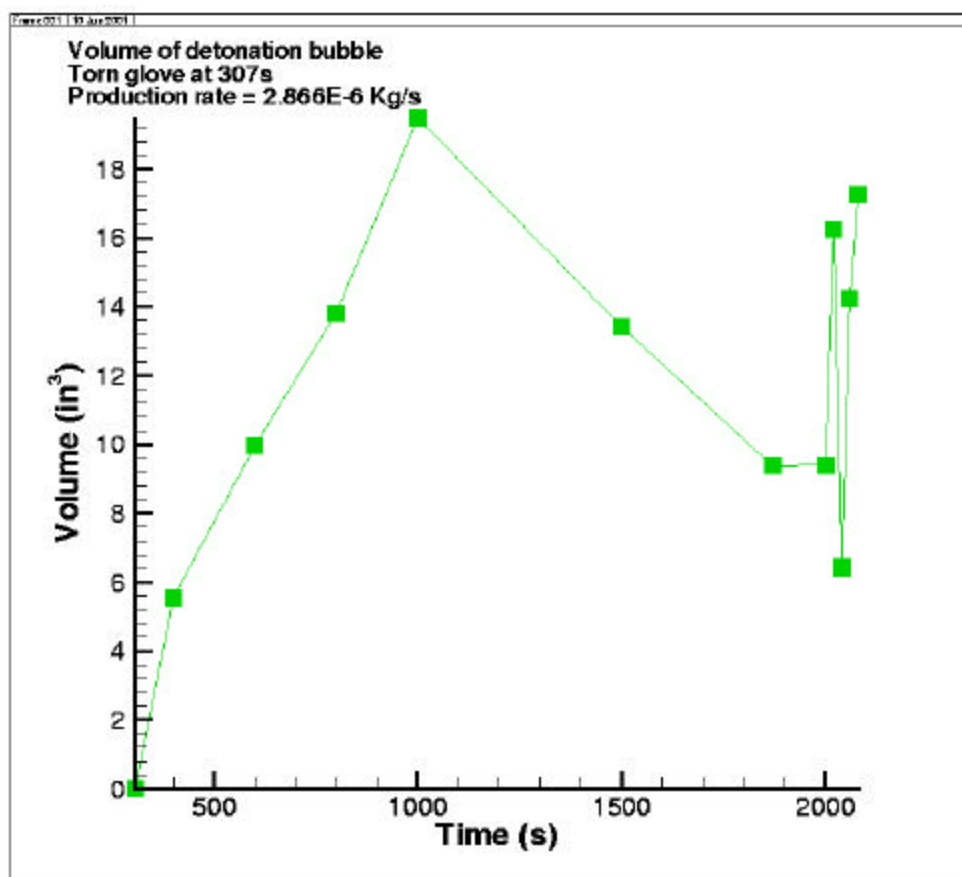


Figure 7 - Variation in Detonable Volume Size for Higher H₂ Production Rate
(data before 1800 s reflects aliasing)

The mean of the values in Fig. 7 is about 12 cubic inches and the highest value is about 19 cubic inches. This is higher than the values for the 1.433 mg/s case, although not twice as high. In fact, the mean values differ by a factor of 1.50 . This would imply a scaling to hydrogen evolution rate of:

$$(dH_2/dt)^{0.585} \propto (\text{detonable volume})$$

With this scaling, the predicted maximum detonable volume for the 9.164 mg/s evolution rate would be about twice that for the 2.866 mg/s case, or 38 cubic inches.

To convert these volumes to standard explosive units, let us consider that the entire volume is a stoichiometric mixture of hydrogen and oxygen, and that it is at a temperature of 400°C. For the 19 cubic inch case, there would be 7.578 mg H₂ in this mixture, with a TNT equivalent of 0.182 g. The 38 cubic inch case would then be equivalent to 0.364 g TNT. Of course, this reaction would be a deflagration instead of the detonation achieved with TNT.

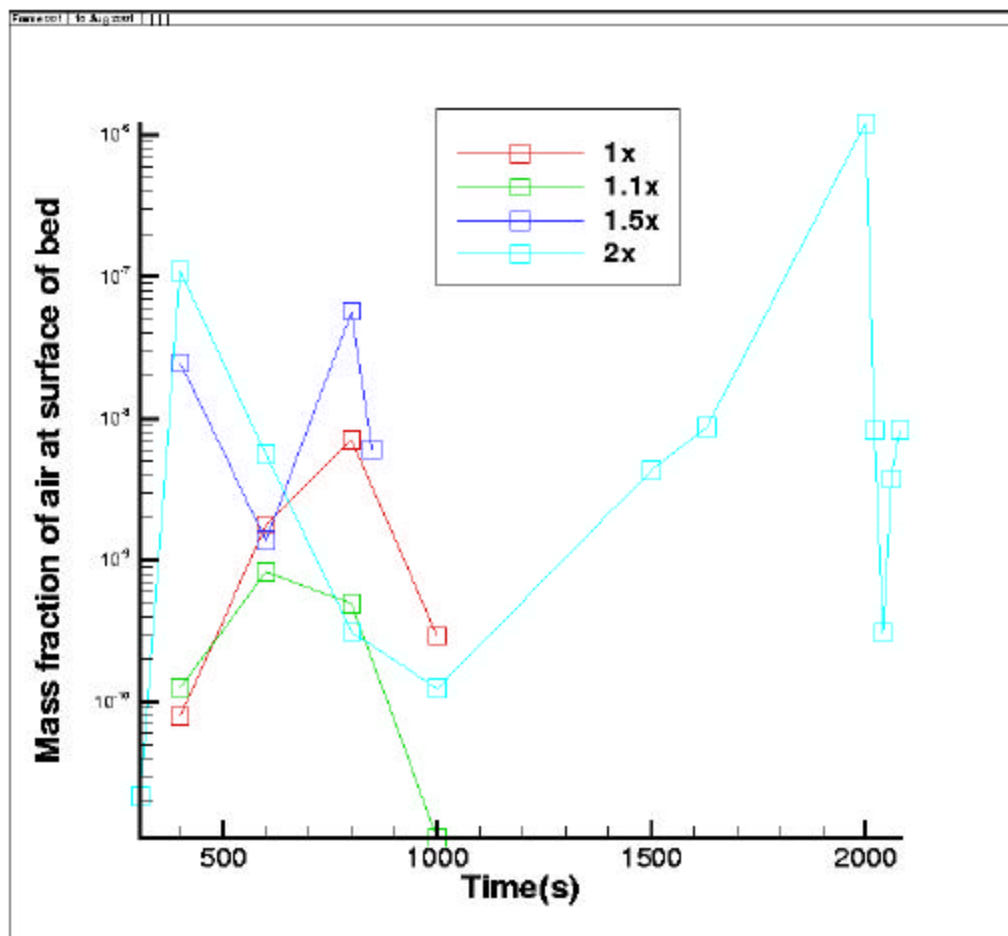


Figure 8 - Comparison of the Air Mass Fraction at the Bed Surface vs Time for a Range of Hydrogen Production Rates from 1.433 (1X) to 2.866(2X) mg/s

Scenario 6C: While it is obvious from Figs. 3-5 that the detonable volume stands off the surface of the bed, that does not imply that no oxygen is getting to the bed surface. It just means that the bottom surface of that volume is more or less at 5 vol % oxygen^{iv}. This could still mean that sufficient oxygen would get to the bed surface to cause sufficient additional heating to change the characteristics of the system. Therefore, a set of runs was performed to estimate the mass fraction of air at the surface of the bed assuming a constant hydrogen evolution rate and no H₂-O₂ explosion. A range of hydrogen production rates was used. It was expected that lower production rates would be associated with higher air mass fractions, and vice versa. This may indeed be true for a statistically robust sample, but Fig. 8 shows only the noisy behavior characteristic of this system. In all cases, however, the mass fraction of air is 10⁻⁶ or considerably less, which should have no practical effect to perturb this system.

In order to demonstrate that this oxygen concentration is truly of no concern, a set of thermochemical calculations was done with HSC Chemistry as follows:

A reaction system was set up for the thermal decomposition of UH₃ using input materials as an equimolar mixture of U metal and UH₃ and output materials as U metal and H₂ gas. An additional input of the exact amount of heat needed to balance the endothermicity of the hydride decomposition was used. This reaction system was then perturbed, by adding controlled amounts of O₂ as an input and U₄O₉ as output.

Such a perturbation increases the temperature of the system due to the heat of oxidation of U metal. A series of final temperatures for the equilibrium reaction system were obtained, using 400°C as the starting temperature and the ratio of O₂ consumed to H₂ evolved as the controlled variable. Results are summarized in Table 2 below.

Table 2 – Impact on Temperature of Adding Oxygen to the Dehydrating Reaction System

Moles O ₂ Consumed / Moles H ₂ Evolved	Final Temperature (°C)
0.00165845	410
0.00272169	420
0.00379410	430
0.00487310	440
0.00595726	450

It must be remembered that this is not a prediction of what will happen, but only a definition of the thermal effect if the reaction proportions are as specified. With that in mind, consider that the ratio of O₂ to H₂ is basically a concentration unit. For example, the second row of the table states that for O₂/H₂ = 0.00272169 the temperature rises from 400 to 420°C; this is equivalent to saying that for an O₂ concentration of 0.27 vol % the only effect is to raise the temperature 20 degrees. That temperature increase would probably suppress the reaction through increased H₂ evolution.

As Figure 8 shows that the air mass fraction is equal to or less than 10⁻⁶, the volume fraction of O₂ at the bed surface would be 1.45*10⁻⁸, or 1.45*10⁻⁶ vol %. Clearly, for as long as the H₂-O₂ mixture does not explode and the evolution rate is maintained, access of O₂ to the bed is minimal.

The remaining area of interest is the question of what conditions can cause the expulsion of bed material out into the glovebox and what are the consequences of such an event.

Scenario 6D: Analysis of Potential Expulsion of Uranium-bearing Particulates from Crucible into Glovebox Space and Development of a Worst-Case Condition

The basic concept for this scenario is that after a glove port opens, a slug of air enters the crucible during a transient condition (perhaps following a H₂-O₂ explosion), reacting quickly with the powder bed which creates heat and a temperature excursion, resulting in generation of large amounts of hydrogen gas from the increased thermal decomposition of UH₃. This rapidly evolving hydrogen could then entrain U, UO_x and UH₃ powder and carry it into the larger glovebox space where it might contact sizeable amounts of air and rapidly combust.

The configuration of the crucible and powder bed for this scenario starts with the 1.5-inch ID MgO crucible filled with UH₃ powder to within 8 inches of the top (as noted earlier, this is more conservative than the now-nominal case with 4 inches). It is assumed that the system is at 400°C and that thermal decomposition has progressed such that a layer of U powder overlays the UH₃ bed. This is a worst case; if there is only UH₃ in this restricted geometry, the UH₃-O₂ reaction tends to suppress itself through generation of gases unless there is complete H₂ combustion, which for reaction to form U₄O₉ and H₂O would even then lead to only a 4.2% drop in moles gas in the crucible (counting the nitrogen content). If there is an overlayer of U powder, there could in principle be a reaction between the U and either O₂ only, or O₂ and N₂, which would result in significant net gas consumption and therefore would not be self-suppressing. The heat generated by this reaction could then be transferred to underlying UH₃, which would respond by endothermically decomposing and generating H₂. This H₂ would expand and tend to entrain particulate matter, thus enabling the said expulsion of uranium material.

There are numerous variables that would have to be specified to fully understand this process:

- the volume of air reacted (and thus the heat liberated) prior to generation of expelling gases;
- the degree of involvement of N_2 in the reaction;
- the proportions of U and UH_3 powders involved in the reactions;
- the total quantity of U and UH_3 powders involved in the reactions;
- the exact stoichiometries of the reactions, their kinetics and thermodynamic properties;
- the thermal conductivities, emissivities and heat capacities of all the materials; and
- the densities of all components and their particle sizes (to estimate entrainment efficiency).

This being a transient and not a steady-state process, the volume of air reacted in the first such burst would be finite. Subsequent reaction following the first burst should be smoother and would probably result in less expulsion of gases and powders, due to the tendency to self-suppress when reacting with UH_3 in a confined space. Estimating the initial reacting air volume is difficult. We will take 250 cc as a working number; that is approximately equal to the free volume in the headspace over the powder bed, plus a little. It is also a typical number for the flammable or detonable volume associated with the H_2 - air mixtures that would form initially after a gross air leak. Explosion of such mixtures could in fact be the precursor to the reaction of air with the powder bed as discussed in this section.

If there was no reactivity of N_2 with U powder, the reaction heat could be partly transferred to N_2 which would expand suddenly but not act to entrain significant powder. If there was reactivity of N_2 with U powder, there would tend to be more air drawn into the crucible due to the loss in numbers of moles of gas. For the calculations in this section, we will assume that air reacts with U to form U_4O_9 and UN in proportion to the composition of air and that all the reaction heat is taken up into the powder bed.

If a rigorous, time-dependant simulation of this process were done, one would start with a H_2 - O_2 explosion and expansion of gases out of the crucible, re-entry of air into the crucible, reaction of U powder with air according to the appropriate kinetic equations and taking account of the heating of the bed by the reaction, transfer of heat to the UH_3 as described by thermal conductivities and heat capacities (as well as loss of heat through radiation and conduction to the covering gas), evolution of hydrogen as described by equilibrium pressure and kinetic equations, and entrainment of particulates as described by the velocity and density of hydrogen as well as the density and cross-section of the U and UH_3 particulates, followed by distribution of the entrained particles into the space above the crucible.

This would be an extremely complex calculational problem, requiring the combination of diffusion, convection, heat, mass and momentum transfer across phase boundaries, and chemical reaction thermochemical and kinetic properties. Because it was seen as a practical impossibility to accomplish this for this project, it was decided to use a series of equilibrium thermochemical calculations to get a feeling for what might happen under certain limiting conditions.

For the data quoted in this section, the reaction and species properties from a previous report^v are used. An Excel spreadsheet calculation was used to fine-tune stoichiometric compositions of the reactions, which was required to permit, for example, reaction to a constant temperature across a range of composition. The reaction heat and final temperature calculations were set up using the HSC Chemistry^{vi} Heat and Material Balance feature, feeding the input quantities from the Excel spreadsheet. Given the size of air bubble (at 400°C) specified as above, a common quantity of oxygen (0.00095075 moles) and the proportionate amount of atmospheric nitrogen was used to react with the powder bed. A starting quantity of 1.05 moles of UH_3 powder was used for all calculations, with one variable being the proportion of U powder in the bed as a result of prior thermal decomposition. An additional set of calculations was run examining the effect of limiting the quantity of bed material exposed to the air

reaction and subsequent thermal effects. This is a reasonable scenario, since heat transfer from reaction at the top of the bed can be expected to require time to propagate downward, during which time accelerated thermal decomposition of UH_3 , H_2 evolution and associated entrainment of powder will be occurring.

By manipulating the amount of H_2 evolved in the simulations, the final temperature can be adjusted as needed in order to demonstrate the effect of composition independent of temperature. This works because, while the air reaction with the bed is exothermic, the UH_3 thermal decomposition is endothermic. Thus, the more H_2 evolved the more cooling of the bed is seen. One final component of the analysis is heat from the furnace. To operate at a steady state temperature during the decomposition process, a certain amount of electric power must be dumped as heat into the system to compensate for the endothermicity of the decomposition. The simulation assumes that 259 Kcal of total extra heat is supplied to the 1.05 moles of uranium hydride/uranium powder. A constant start temperature of 400°C is assumed.

The first comparison in Table 3 assumes a constant final temperature of 431.2°C, which is almost equal to the temperature at which the hydrogen pressure over the hydride is 1.00 atmosphere. Note that the evolved hydrogen quantity required becomes larger at higher proportions of U relative to UH_3 . This is because U has a lower heat capacity than UH_3 . A total uranium quantity of 1.05 moles is assumed.

Table 3 – Effect of Composition on H_2 Evolution Required to Hold at Specific Temperatures

UH_3 (moles)	U (moles)	Final Temperature (deg C)	H_2 Evolved (moles)
0.20	0.85	431.2	0.02975
0.50	0.55	431.2	0.02730
0.80	0.25	431.2	0.02510
0.20	0.85	470.2	0.01000
0.50	0.55	470.2	0.00465
0.80	0.25	468.8	0.00000

The second comparison looks at the amount of H_2 cooling required to control the final temperature T_f to approximately 470°C. Note that significantly less H_2 evolution is required compared with holding T_f to 431.2°C; and that again the presence of higher amounts of UH_3 permits limiting the temperature rise with less H_2 evolution.

The data in Table 4 illustrate, for the same proportions of UH_3 and U, the temperatures that will be achieved with zero H_2 cooling as well as the equilibrium H_2 pressures that will exist over UH_3 at these temperatures.

Table 4 – Effect of Composition with Zero H_2 Evolution

UH_3 (moles)	U (moles)	Final Temperature (deg C)	P_{eq} (atm)
0.20	0.85	489.7	3.06
0.50	0.55	478.0	2.48
0.80	0.25	468.8	2.10

The comparison in Table 4 again illustrates the effect of the greater heat capacity of UH_3 in moderating the temperature rise. The higher equilibrium H_2 pressure associated with the higher temperature can be considered as having a higher “potential” for blowing powder out of the crucible.

It is clear from considering the results in Tables 3 & 4 that one element in the specification of worst-case conditions is a relatively low UH_3/U ratio in the part of the bed affected by the reaction with air. This cannot be carried too far, because in the limit of zero UH_3 there would be no gas source to blow out the powder. The next step is to consider, for a low UH_3/U ratio, the effect of changing the total quantity of bed material that is involved in absorbing the heat generated by the air-U reaction. For this comparison, molar proportions of 20% UH_3 , 80% U are assumed, as well as uniform H_2 cooling to 470°C . Calculations are performed based on a range of total ($\text{UH}_3 + \text{U}$) moles. The total moles of evolved H_2 required to cool the specified bed material quantity to 470°C is listed in Table 5, as well as the pressure P_c that this amount of H_2 would generate at that temperature within the 230-cc crucible headspace (which should be related to the driving force to blow out material). The use of a 4-inch headspace instead of the 8-inch headspace would change the absolute values, but not the relation between values on which the analysis is based.

Other elements in this table require explanation. As is discussed in an earlier report,^{vii} the force \mathbf{F} exerted on a body by wind varies as the 4th power of the velocity, and for turbulent flow the velocity varies as the square root of the pressure. Thus:

$$\mathbf{F} \propto (P^{0.5})^4 = P^2,$$

and therefore the tendency for a gas source to blow particulates out will be proportional to the square of the pressure of that source. The final factor in this is the availability of particulates; the more in the path of the gas stream, the more one can expect to be entrained. The measure of this is the fraction of total material (# moles M) involved in absorbing reaction heat. So with the factors described, an index \mathbf{I} can be defined which will describe the relative amount of powder carried into the space above the crucible under various conditions:

$$\mathbf{I} = P_c^2 * M.$$

Conditions yielding maximum values of \mathbf{I} should yield maximum amounts of powder blown into the space above the crucible.

Table 5 – Relative Tendency to Blow Powder out of Crucible (20% UH_3 , 470°C)

Total Moles M	Moles H_2	H_2 Pressure P_c (atm)	Index \mathbf{I}
1.05	0.010	2.65	7.374
0.35	0.0251	6.655	15.501
0.10	0.030	8.05	6.480

So, this chain of reasoning has led us to consider that if about 1/3 of the total bed is involved with taking up heat from the reaction with air, and that a small (but not too small) percentage of that is UH_3 , We will have a worst case.

It is further possible to refine this conclusion by taking the above worst case (0.35 moles, 20% UH_3) and calculating the actual temperature and pressure that one might expect within the crucible, given that the pressure in the crucible should equal the equilibrium pressure over the hydride at the final temperature. Manually iterating Excel and HSC Chemistry as before, one finds the following self-consistent values:

$$T_f = 515.4^\circ\text{C}$$

$$P_c = P_{eq} = 4.74 \text{ atm}$$

$$\text{H}_2 \text{ evolved} = 0.017 \text{ moles}$$

The most important conclusion out of this is that one might expect as a worst case about 1/3 of this powder bed to be blown out of the crucible. This has implications for calculations of the energy in possible subsequent reactions of the entrained powder.

Of the powder that may be blown into contact with air, some will be preoxidized to uranium oxide, some will be uranium metal, and some will be UH_3 . We have said that the worst case for dispersing powder appears to be when 0.35 moles of the total 1.05 moles is involved, and of that when 20% of the moles are UH_3 . It is a reasonable estimate that a maximum of 10% of the theoretical energy for combustion of a cloud of dispersed particles will be realized. Therefore, the fraction of energy **Fr** from the combustion of UH_3 that may be actually obtained may be described by:

$$\mathbf{Fr} = (0.35/1.05) * (0.2) * (0.1) = 0.0067 \text{ (or 0.67\%) .}$$

It must be remembered that details of this analysis including the values quoted for combustion efficiency do hinge on the choice of 250 cc as the volume of air reacting with the U powder bed overlayer. However, the general conservatism of this analysis should compensate for that uncertainty.

The reaction of U metal powder with air would add further energy to the combustion system. However, there are factors which would reduce this contribution: (1) the U particulates should be less finely structured than the hydride, having been sintered slightly (and slightly passivated) in the course of the initial in-crucible oxidation; (2) such a reduction in available area (and partial passivation) should reduce the rate of reaction such that heat is generated over a longer time and hence has less shock impact; and (3) U metal is so reactive that it can react with nitrogen as well as with oxygen. Since all the products of reaction of U with oxygen and nitrogen are solids in the temperature range of interest, in the limit of complete reaction there would be no positive pressure pulse and indeed there would be a negative pressure generated. The worst case would be for partial reaction, heating up the unreacted gases to create a positive pressure pulse. It is difficult to predict without experiments just what would happen. It does seem likely that kinetic and mass transfer barriers would slow the release of energy to the point where the contribution of U particulates to an explosion would be minimal. However, the possibility of synergism between the hydride and metal combustion processes cannot be 100% ruled out. Either a very sophisticated (and expensive) simulation of this potential dust explosion, or experimental testing, would be required to be totally sure of the result. For the time being the probability seems good that the calculation of **Fr** above, together with the blast effect calculations described later in this report, will adequately describe the potential for damage from this postulated event.

Scenario 7: Analysis of the Effect on Glovebox Integrity of Hydrogen and UH₃ Explosions in Air

The full description of the calculations of this effect is given in the memorandum from David Sulfredge to Jon Bullock which is reproduced here as Appendix A. The main conclusions, as well as some additional discussion, are given in this section.

These calculations assume that there has been a massive air leak such as has been described earlier, leading to an atmospheric composition in the glovebox approaching that of air, followed by a dispersion of combustible material into that atmosphere. The dimensions of the glovebox were taken into account. The enthalpy of reaction of the dispersed material with oxygen was calculated using HSC Chemistry on two bases: (1) assuming that all the hydrogen content of the hydride was available as hydrogen gas, which reacted with a stoichiometric amount of oxygen to form water vapor; and (2) assuming that the UH₃ particulates were dispersed and reacted with oxygen to form U₄O₉ and water vapor. The UH₃ reaction is considerably more energetic, but even with hydrogen gas only 10% combustion efficiency is seen for scenarios like this; with UH₃ there should be considerable kinetic and mass transfer barriers to realizing energy release on a rapid time scale. Reaction of U metal powder with air is not considered here.

The Sulfredge calculations used the theoretical enthalpy releases for these two reactions and determined the impact on the box structure. Multiple calculations were performed, using various fractions of the theoretical explosive yield to simulate various combustion efficiencies. The detonation model was used, as there are quantitative methods to relate detonation energy to impulse transferred to the surroundings. However, the conditions in this combustion system will result in deflagrations rather than detonations, with considerably lower effects on structures. A key calculated result was the initial velocity of the window as a result of the impulse from the postulated explosion. This has to be interpreted in light of other factors which are not considered in the current calculation: (1) the restraint from the window clamp will retard motion and tend to allow pressure venting through the open glove port as well as possibly around the window at points that come free of the clamp while the rest of the clamp is holding (one consequence of the slower speed of a deflagration is the possibility of venting pressure); (2) the calculation yields the instantaneous velocity, and as soon as there is significant motion air resistance will tend to slow down the velocity at longer times; and (3) because the window orientation is at an angle to the vertical, gravitational acceleration will act to slow any vertical component of velocity.

Table 3 of Appendix A lists for the H₂ combustion case the impulse applied to the window and the resultant initial velocity, assuming a window thickness of ¼ inch and consequent mass of 9.34 Kg (higher thicknesses and masses will result in lower velocities). A curvefit of the efficiency-velocity data indicates that at an efficiency of 0.67% an initial velocity of 3.99 m/s would be obtained. Considering that this is probably an excessively artificial case (the mechanism of getting all the hydrogen extracted and in the glovebox atmosphere is unknown), the UH₃ combustion results are more pertinent. In that case, for 0.67% the curvefit indicates an initial velocity of 6.025 m/s.

Taking the angle of the window into account, the velocity of the window in the gravity field is described by:

$$V(t) = V_o - (g * \cos(61.4 \text{ deg})) * t ,$$

which predicts that for an initial velocity of 6.025 m/s the vertical component of window velocity would drop to zero at a height of 3.866 m and that it would take 1.2834 s to get there. It must be emphasized that the constraint of the window clamp, loss of impulse energy to leakaround, and air resistance is not in this calculation. The fact that this is really a deflagration and not a detonation will also lower the pressure wave intensity, probably by a factor of two. The resulting actual performance to move the window should be significantly less, and probably not enough to cause significant equipment or structural damage.

However, these will not be trivial forces with respect to human safety. During a time when such a scenario is possible (i.e., if a massive air leak were to occur), personnel should be sheltered from a direct line of sight to the front of the glovebox for a prudent distance.

A remaining issue relates to the likelihood that the MgO crucible might fracture due to an explosion and disperse more material to yield a more serious contamination problem or possibly another explosion hazard. Even at 20% combustion efficiency for the UH_3 case, which could produce 392 psi overpressures at the crucible, a hoop stress calculation for the crucible wall yields only 1177 psi. This can be compared to a literature value^{viii} of 36 Ksi tensile strength for MgO. With these values, it seems very unlikely that the crucible would break during any creditable explosion in the glovebox.

CONCLUSIONS

Several types of hazards associated with operation of a thermal decomposition process for uranium hydride were analyzed. The concentration of hydrogen in the argon purge exit gas was found to be of no concern *re* flammability within wide operating limits and even if the purge was lost. The additional hazards associated with a massive ingress of air during operation were examined in detail. The joint presence of H_2 and O_2 in regions of space was evaluated as the product of the O_2 mole fraction and the square of the H_2 mole fraction. Calculated values of this function were compared with the values obtained from the limits for flammability and detonability for H_2 in air, and the volumes of the explosable mixture estimated. Assuming the entire explosable volume to be stoichiometric H_2-O_2 , it appears that for the conditions used in the present analyses, the explosive potential in H_2-O_2 mixtures would be on the order of less than 0.4 gram TNT equivalents. If the furnace is disengaged either by interlock or administrative control at the time that the argon purge stops and the glove port opens, cooling might be rapid enough to remove the potential for ignition of the gas mixture before either limit is reached. There may be the better part of a minute to work with in turning off furnace power and other ignition sources before an explosive mixture develops. However, it may be unrealistic to expect to cool the powder bed sufficiently to avoid energetic reaction with air.

Alternatively, a strategy might be pursued in which power remained on to keep the hydrogen evolving, and thus keep the air away from the powder bed, until most or all of the hydride was decomposed. The rationale for this is that the energy in a creditable dust explosion involving UH_3 dispersed into the glovebox could be as high as 2 grams TNT equivalents, or 5 times that estimated for the hydrogen explosion. On the other hand, if the hydrogen continues to be evolved during a time when there is a massive air leak, a H_2-O_2 explosion, although of small energy, may set up the system for subsequent dispersal of UH_3 and thus a possibly larger explosion. The case where a massive leak at a glove port occurs, but the 50 cfh argon purge continues, was not explicitly analyzed, but in our judgement the air inleakage would be slow enough that shutdown and cooling could be done in an orderly, non-crisis manner. It is judged prudent to evacuate personnel from the immediate vicinity of the glovebox, especially in front of the window, during a time when any of the upset conditions that involve significant air ingress exist, and until they have run their course.

Appendix A – Sulfredge Memo

Date: August 3, 2001

To: Jonathan S. Bullock

From: C. D. Sulfredge

cc: G. E. Giles and M. W. Wendel

Subject: Calculated Parameters for Potential Hydrogen and Uranium Hydride Explosions
in a Glove Box

For this study, I was asked to calculate the overpressures and transmitted impulses associated with the largest possible hydrogen and uranium hydride explosions inside a glove box. The glove box has the cross-sectional shape and dimensions shown in Fig. 1, with a total length of 97" in the direction extending into the paper. On the sloped face of the box is a viewing window that is 4" less tall than the slanted area and 6" less wide. One of the major objectives of this work is to calculate the potential explosive impulse incident on this window and the velocity at which it might be blown out. The window consists of Plexiglas or Lexan plastic with a density of 1.19 g/cm^3 , and will be assumed to have a conservatively low thickness of 1/4 inch. This assumption leads to a window mass of 9.34 kg.

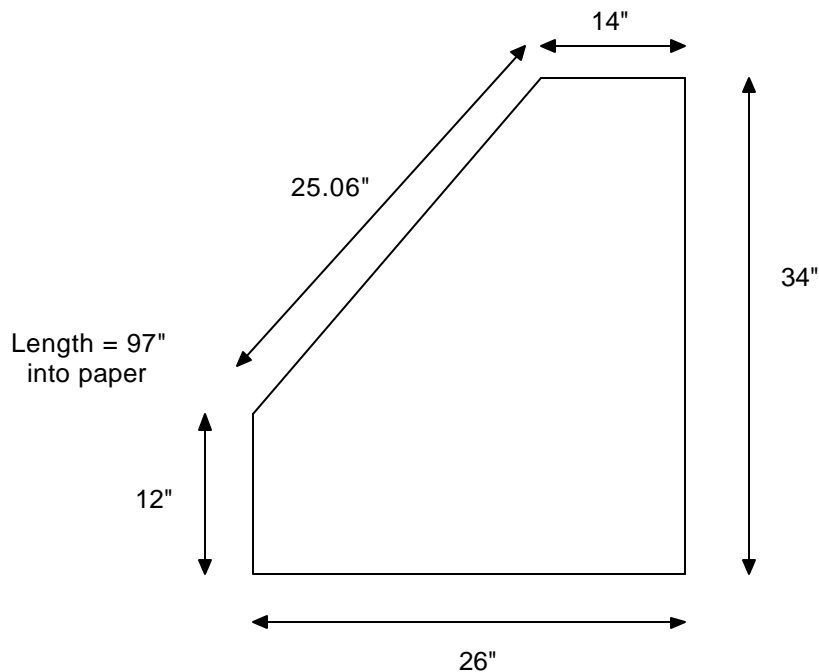


Figure 1. Cross-sectional View of the Glove Box

The detonation point for the hydrogen or hydride mixture will be assumed to be centered within the glove box and 22" above the bottom. For purposes of calculating incident overpressures on the ends, back, top, and bottom planes of the box, this leads to the stand-off distances summarized in Table 1. An accurate calculation of the overpressure and impulse incident on the window requires dividing it into several panels to capture spacial variations in the blast parameters. Figure 2 shows the panelization scheme chosen. There are a total of 7 subsections, with Panel 1 centered directly in front of the assumed burst point. Since the situation is symmetric about the midplane of the box, Panel 4, #1 and Panel 4, #2 (as well as Panel 5, #1 and Panel 5, #2) will experience equal blast parameters. Thus

blast conditions have to be calculated on only 5 different panel segments of the window for each case analyzed. Table 2 lists the surface areas and distances to the blast center used for Panel Segments 1-5.

Wall	Stand-off Distance (in)
Ends	48.5
Back	13
Top	12
Bottom	22

Table 1. Distances from Glove Box Walls to Blast Center

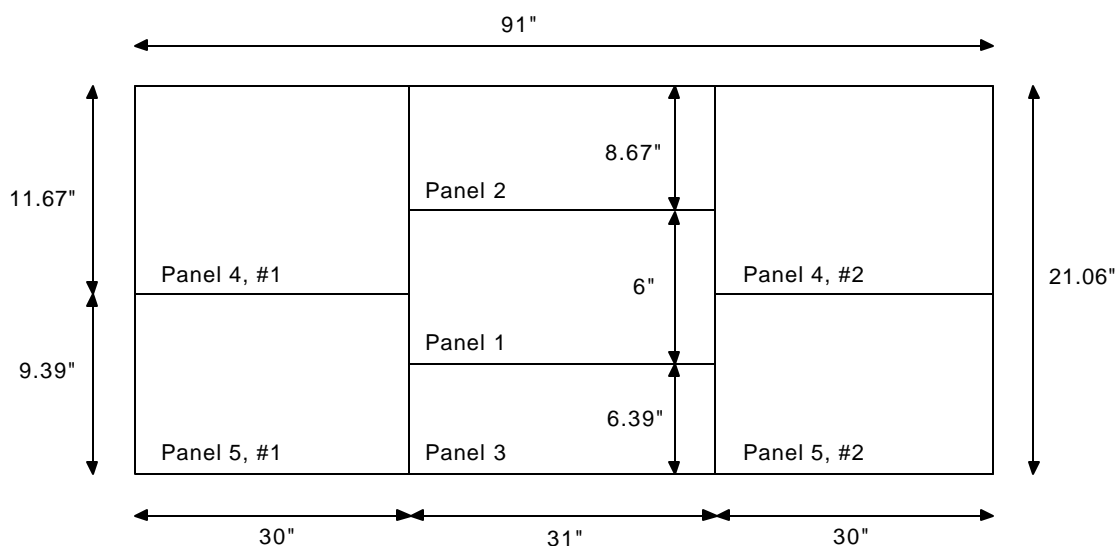


Figure 2. Illustration of the Glove Box Window Panelization

Panel Segment	Number Present in Window	Surface Area (in ²)	Distance from Expected Blast Center (in)
1	1	186.0	7.55
2	1	268.77	7.60
3	1	198.09	11.84
4	2	350.1	31.29
5	2	281.7	32.30

Table 2. Summary of Window Panelization Data

Calculation of the impulse and overpressure was done for both hydrogen and uranium hydride reactions. The H_2 calculation assumes 3.125 g of H_2 is available for immediate reaction and analyzes the effects for combustion efficiencies of 0.25%, 1%, 2.5%, 5%, 10%, 15%, and 20%. The equivalent TNT charge weight corresponding to each efficiency is determined by starting from 1g $H_2 = 24g$ TNT and reducing the blast output by the appropriate

reaction efficiency. Then the potential for enhancement of the impulse and overpressure due to confinement of the explosion within the glove box must be checked [1]. If any of the box walls or the window is within a characteristic distance of the blast center, the equivalent TNT charge must be increased before obtaining the impulse and overpressure from the standard TNT tables. The characteristic dimension within which a charge is considered “confined” by one or more walls gets larger as the charge increases, so the enhancement check must be repeated at each efficiency level.

For the hydrogen reactions, even the 20% efficiency case was too small an explosion to experience enhanced yield due to confinement in the center of the glove box. Thus the overpressures and impulses can be obtained directly from the standard free-field blast tables for TNT charges [2]. Results for the 3.125 g H₂ reaction at all 7 efficiency levels are given in Table 3. Peak overpressures are provided for the window on Panel 1 (which experiences the highest overpressure) and on the remaining surfaces of the glove box.

Efficiency	TNT Equiv. Weight (g)	Peak Overpressure on Surfaces (psi)	Total Impulse to Window (N sec)	Initial Window Velocity (neglecting clamp) (m/sec)
0.25%	0.1875	Window Panel 1 – 9.30 Ends – 0.59 Back – 3.26 Top – 3.76 Bottom – 1.47	26.167	2.8
1%	0.75	Window Panel 1 – 26.3 Ends – 0.98 Back – 7.84 Top – 9.27 Bottom – 2.93	41.935	4.5
2.5%	1.875	Window Panel 1 – 53.7 Ends – 1.43 Back – 15.2 Top – 18.3 Bottom – 5.04	55.038	5.9
5%	3.75	Window Panel 1 – 90.8 Ends – 1.97 Back – 25.9 Top – 31.1 Bottom – 8.01	64.879	6.9
10%	7.5	Window Panel 1 – 151.3 Ends – 2.82 Back – 44.4 Top – 53.6 Bottom – 13.2	72.088	7.7
15%	11.25	Window Panel 1 – 201.6 Ends – 3.53 Back – 60.9 Top – 72.9 Bottom – 17.9	77.803	8.3
20%	15.0	Window Panel 1 – 245.9 Ends – 4.20 Back – 75.6 Top – 90.6 Bottom – 22.3	82.532	8.8

Table 3. Peak Pressure and Impulse Results from Hydrogen Reactions

The total integrated impulse delivered to the window is obtained by summing over all panel segments of the window. This total impulse is then set equal to the change in momentum experienced by the window. Since momentum can be expressed as mass multiplied by velocity, one can solve for the initial velocity at which the window might be blown out. This analysis assumes the window comes out as a single unit rather than fragmenting and neglects any retarding action of the window clamps (which is conservative). Calculated initial window velocities for the 1/4" thickness ranged from 2.8 m/sec up to 8.8 m/sec as the hydrogen combustion efficiency changed from 0.25% to 20%. Using a 3/8" thick window would multiply all these velocities by a factor of 2/3 due to the increase in window mass, leaving all the calculated overpressures and impulses unchanged.

A similar set of calculations was done to obtain TNT equivalent weights for the uranium hydride reaction. The 3.125 g of hydrogen corresponds to 1.0335 mol of UH_3 available to react. Based on the HSC Chemistry V.4 calculations provided, the reaction energy is about 1300 kcal/(4 mol UH_3). The standard heat of reaction for TNT is 1100 cal/g [2]. Therefore, carrying out the unit conversions shows that the maximum equivalent TNT charge (in g) for the hydride reactions would be given by 305.35 multiplied by the assumed efficiency factor. Calculation of the hydride TNT equivalents and associated blast parameters has also been conducted at 0.25%, 1%, 2.5%, 5%, 10%, 15%, and 20% combustion efficiencies, and the results are summarized in Table 4. This is a considerably more energetic reaction than the one involving hydrogen, and for 15% and 20% efficiencies the potential explosion is large enough that one has to include the effect of glove box confinement on the impulse and overpressure. For these two hydride efficiency cases, the equivalent TNT charge weight must be enhanced by an additional factor of 2 before entering the standard free-field TNT tables. However, given that a uranium hydride reaction involves burning of solid particles, achieving an efficiency >10% would be quite unlikely in any realistic accident scenario. The calculated initial velocities for a 1/4" thick window displaced by the uranium hydride reaction ranged from 4.5 m/sec to 13.1 m/sec for the efficiencies studied in Table 4. As with the hydrogen cases, changing to a 3/8" thick window would multiply all these velocities by 2/3. Velocities would also be reduced by any energy expended in breaking the clamps.

The calculations described in this report should be quite conservative compared to realistic accident scenarios inside the glove box for multiple reasons. First of all, it is very unlikely that the entire 3.125 g of H_2 or equivalent amount of UH_3 would ever be available for instantaneous reaction at any one time. The mixture of H_2 or UH_3 with air almost certainly would be inhomogeneous and not in a stoichiometric ratio. Any realistic ignition mechanisms for the mixture in the glove box would be similarly inefficient, especially for the solid particle reactions involving UH_3 . Combustion efficiencies of up to 20% have been observed for stoichiometric hydrogen/oxygen mixtures ignited by small pentolite charges [3]. Thus 20% overall efficiency represents almost an absolute upper limit on the realistic reactions in an accident. In any realistic accident scenario, 5% efficiency is probably about the greatest value likely to be observed.

Either the hydrogen or hydride reaction actually involves a deflagration (or rapid burning) rather than the detonation behavior characteristic of a high explosive like TNT. Although point-source detonation blast wave theory is not particularly well suited to analyzing deflagration, there is no better general methodology available for such cases [4]. Compared to high explosives, deflagrations tend to be distributed over an extended volume and give off larger amounts of gas at a much slower rate. The corresponding blast waves from deflagrations have far less sharp overpressure spikes than detonations and are more spread out in time. Thus the peak overpressures on surfaces calculated from a detonation model in this report should be highly conservative.

The overall impulse delivered to surfaces by a deflagration will be similar to the corresponding detonation, but it will take longer to be applied. In a deflagration, the pressure build-up would be slow enough that the glove box window would probably begin to move (venting the pressure behind it) before the full impulse calculated from detonation theory had time to be applied. Thus the predicted velocities at which the glove box window might be blown out are likely to be quite conservative in realistic accident scenarios. Any clamping arrangement sufficiently strong to secure the window against even its own weight would also absorb a significant portion of the deflagration impulse before the window came free, introducing an additional element of conservatism. Finally, the sloped surface of the glove box is oriented at an angle of about 61.4 degrees to the horizontal, so $9.34 \text{ kg} \cdot (9.81 \text{ m/sec}^2) \cdot \cos(61.4 \text{ deg.}) = 43.9 \text{ N}$ of the window's weight will also help hold it in place against any potential internal explosions.

Deflagration phenomena like those involved in the potential accidents inside the glove box are clearly inherently complex problems depending on many different variables that are all subject to a considerable degree of uncertainty. To completely define the problem, one would have to specify the precise amount of reactants, the geometry of the system, and the ignition mechanism, all of which depend heavily on the specific accident scenario chosen. The exact method used to secure the glove box window would also be very important. A great deal of effort, and possibly even some scaled experimental testing, would be required to do a rigorous analysis of the effects for a specific accident scenario inside the glove box.

Efficiency	TNT Equiv. Weight (g)	Peak Overpressure on Surfaces (psi)	Total Impulse to Window (N sec)	Initial Window Velocity (neglecting clamp) (m/sec)
0.25%	0.7634	Window Panel 1 – 26.6 Ends – 0.99 Back – 7.94 Top – 9.39 Bottom – 2.96	42.177	4.5
1%	3.0535	Window Panel 1 – 80.4 Ends – 1.81 Back – 22.1 Top – 26.5 Bottom – 6.96	62.049	6.6
2.5%	7.6338	Window Panel 1 – 153.2 Ends – 2.85 Back – 45.0 Top – 54.3 Bottom – 13.4	72.248	7.7
5%	15.27	Window Panel 1 – 249.0 Ends – 4.25 Back – 76.6 Top – 91.8 Bottom – 22.6	82.822	8.9
10%	30.535	Window Panel 1 – 393.2 Ends – 6.63 Back – 128.3 Top – 152.8 Bottom – 38.7	94.068	10.1
15%	45.803	Window Panel 1 – 766.1 Ends – 14.5 Back – 277.7 Top – 326.0 Bottom – 89.9	116.676	12.5
20%	61.07	Window Panel 1 – 898.6 Ends – 18.1 Back – 336.3 Top – 392.3 Bottom – 111.5	122.370	13.1

Table 4. Peak Pressure and Impulse Results from Hydride Reactions

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Edwards, E. R.
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Hamby, R. S./Fugate, R. A.
Insalaco, J. W.
Joplin, J. R./ Watkins, J. D.
Lamberti, V. E.
Morrell, J. S.
O'Hara, J. M./Calfee, M. T.
Reiner, R. H.
Simon, K. F.
Sipes, J. E.
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Giles, G. E., Jr. (2)
Sulfredge, C. D. (2)
Wendel, M. W. (2)

Idaho National Engineering and Environmental Laboratory

Bratton, R. L.
Dahl, C. A